

1,2-Diphenylhydrazine  
122-66-7 | DTXSID7020710

Model Performance

|       |      |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.84            | 0.55 | 0.85           | 0.53 | 0.83       | 0.64 |

Model Results

Predicted value: 38.7

Global applicability domain: Inside

Local applicability domain index: 4.53e-01

Confidence level: 5.69e-01

Nearest Neighbors from the Training Set

|  |  |  |
|--|--|--|
| <div>Image not found</div> <div>N,N-Diethylaniline</div> <div>Measured: 102</div> <div>Predicted: 12.8</div>                   | <div>Image not found</div> <div>Isoamyl ether</div> <div>Measured: 170</div> <div>Predicted: 137</div> | <div>Image not found</div> <div>Isoprocab</div> <div>Measured: 8.91</div> <div>Predicted: 13.6</div> |
| <div>Image not found</div> <div>2-(Thiocyanomethylthio)benzothiazole</div> <div>Measured: 209</div> <div>Predicted: 13.0</div> | <div>Image not found</div> <div>Isophorone</div> <div>Measured: 2.00</div> <div>Predicted: 3.19</div>  |  |